George B Bacskay

List of Publications by Year
in descending order

54 papers	1,616 citations	236925 25 h-index	302126 39 g-index
54 all docs	54 docs citations	54 times ranked	1311 citing authors

#	Article	IF	Citations
1	Pyrolysis of Furan:Â Ab Initio Quantum Chemical and Kinetic Modeling Studies. Journal of Physical Chemistry A, 2000, 104, 1861-1875.	2.5	102
2	Spectroscopic constants of the XÌƒ(1A1), Ã£(3B1), and Ãƒ(1B1) states of CF2, CCl2, and CBr2 and heats of formation of selected halocarbenes: An ab initio quantum chemical study. Journal of Chemical Physics, 2000, 112, 2227-2238.	3.0	90
3	The infrared absorption intensities of the water molecule: A quantum chemical study. Journal of Chemical Physics, 1986, 84, 5715-5727.	3.0	88
4	Ab Initio Quantum Chemical and Kinetic Modeling Study of the Pyrolysis Kinetics of Pyrrole. Journal of Physical Chemistry A, 1999, 103, 3923-3934.	2.5	69
5	Homogeneous Conversion of Methane to Methanol. 2. Catalytic Activation of Methane bycis-andtrans-Platin:Â A Density Functional Study of the Shilov Type Reaction. Journal of the American Chemical Society, 2000, 122, 2041-2052.	13.7	62
6	Heats of Formation of Hydrofluorocarbons Obtained by Gaussian-3 and Related Quantum Chemical Computations. Journal of Physical Chemistry A, 2000, 104, 7600-7611.	2.5	60
7	Decomposition of the Benzyl Radical:â€‰ Quantum Chemical and Experimental (Shock Tube) Investigations of Reaction Pathways. Journal of Physical Chemistry A, 1997, 101, 7105-7113.	2.5	59
8	A quadritically convergent hartree-fock (QC-SCF) method. Application to open shell orbital optimization and coupled perturbed hartree-fock calculations. Chemical Physics, 1982, 65, 383-396.	1.9	55
9	A Gaussian-2 Quantum Chemical Study of CHNO:â€‰ Isomerization and Molecular Dissociation Reactions. Journal of Physical Chemistry A, 1999, 103, 6624-6631.	2.5	55
10	Hydrogen bonded complexes of HCl with CO, C2H2, C2H4, PH3, H2S, HCN, H2O and NH3. Molecular Physics, 1992, 77, 61-73.	1.7	54
11	Ab Initio Quantum Chemical Studies of the pKa's of Hydroxybenzoic Acids in Aqueous Solution with Special Reference to the Hydrophobicity of Hydroxybenzoates and Their Binding to Surfactants. Journal of Physical Chemistry B, 1998, 102, 1938-1944.	2.6	53
12	The prediction of nuclear quadrupole moments fromabinitioquantum chemical studies on small molecules. II. The electric field gradients at the17O,35Cl, and2H nuclei in CO, NO+, OHâ¯, H2O, CH2O, HCl, LiCl, and FCl. Journal of Chemical Physics, 1987, 87, 416-423.	3.0	45
13	The Mechanism of Covalent Bonding. Journal of Chemical Education, 1997, 74, 1494.	2.3	44
14	The Virial Theorem and Covalent Bonding. Journal of Physical Chemistry A, 2018, 122, 7880-7893.	2.5	43
15	Characterization of the Ãƒ(1Aâ€³) state of HCF by laser induced fluorescence spectroscopy. Journal of Chemical Physics, 1999, 110, 11277-11285.	3.0	40
16	Heats of formation of phosphorus compounds determined by current methods of computational quantum chemistry. Journal of Chemical Physics, 2002, 117, 11175-11187.	3.0	40
17	An Ab Initio Quantum Chemical and Kinetic Study of the NNH + O Reaction Potential Energy Surface:â€‰ How Important Is This Route to NO in Combustion?. Journal of Physical Chemistry A, 2003, 107, 6792-6803.	2.5	40
18	Covalent Bonding: The Fundamental Role of the Kinetic Energy. Journal of Physical Chemistry A, 2013, 117, 7946-7958.	2.5	40

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19	The electronic spectroscopy of jetâ€cooled difluorocarbene (CF2): The missing Ãƒâ€state stretching frequencies. Journal of Chemical Physics, 1995, 103, 4476-4483.	3.0	38
20	Quantum chemical studies of the pyrrole-water and pyridine-water complexes. Molecular Physics, 1995, 85, 573-585.	1.7	32
21	Abinitioquantum chemical study of the molecular and spectroscopic (infrared and Raman) properties of sulfur dioxide: Comparison with ozone. Journal of Chemical Physics, 1988, 89, 5721-5730.	3.0	31
22	Ab Initio Quantum Chemical and Experimental (Shock Tube) Studies of the Pyrolysis Kinetics of Acetonitrile. Journal of Physical Chemistry A, 1999, 103, 1054-1072.	2.5	31
23	Quantum chemical studies of the potential energy surfaces and vibrational frequencies of the??(1A?),ï¿½(3A?), andï¿½(1A?) states of CHCl and CFCl. International Journal of Quantum Chemistry, 2000, 76, 297-305.	2.0	31
24	An ab initio quantum chemical study of the hydrogenâ€and â€˜â€˜antiâ€™â€™â€hydrogenâ€bonded HF/ClF and HF/Cl2 dimers. Journal of Chemical Physics, 1987, 87, 535-544.	3.0	30
25	Electronic spectroscopy and ab initio quantum chemical study of the Ãƒ(1Aâ€³)â†'XÌƒ(1Aâ€²) transition of CFBr. Journal of Chemical Physics, 1998, 109, 2220-2232.	3.0	29
26	Stabilities, Excitation Energies, and Dissociation Reactions of CF2Cl2and CF2Br2:Â Quantum Chemical Computations of Heats of Formation of Fluorinated Methanes, Methyls, and Carbenes. Journal of Physical Chemistry A, 2000, 104, 11212-11219.	2.5	25
27	Ab Initio Quantum Chemical Studies of the Formaldiminoxy (CH2NO) Radical:Â 2. Dissociation Reactions. Journal of Physical Chemistry A, 1999, 103, 4514-4524.	2.5	24
28	Ab Initio Quantum Chemical Studies of the Formaldiminoxy (CH2NO) Radical:Â 1. Isomerization Reactions. Journal of Physical Chemistry A, 1999, 103, 4505-4513.	2.5	22
29	The Role of Phosphorus Dioxide in the H + OH Recombination Reaction:â€‰ Ab Initio Quantum Chemical Computation of Thermochemical and Rate Parameters. Journal of Physical Chemistry A, 2002, 106, 1533-1541.	2.5	21
30	Quantum Chemical Characterization of theXÌƒ(¹Aâ€²),aÌƒ(³Aâ€²â€²) andAÌƒ(¹Aâ€²â€²) States of CHBr and CHI and Computed Heats of Formation for CHI and CI^{â€}. Journal of Physical Chemistry A, 2010, 114, 8625-8630.	2.5	21
31	Resonance-Enhanced 2-Photon Ionization Scheme for C₂ through a Newly Identified Band System: 4³Î_gâ€“a³Î_u. Journal of Physical Chemistry A, 2015, 119, 12102-12108.	2.5	20
32	Oxidation of CO by SO2:â€‰ A Theoretical Study. Journal of Physical Chemistry A, 2005, 109, 2019-2025.	2.5	19
33	The role of electrostatics in molecular interactions: prediction of shapes and electronic properties of weakly bound complexes. International Reviews in Physical Chemistry, 1986, 5, 139-146.	2.3	18
34	The Basics of Covalent Bonding in Terms of Energy and Dynamics. Molecules, 2020, 25, 2667.	3.8	18
35	Ab initio potential energy surface and vibrational frequencies of HCN. Molecular Physics, 1993, 79, 819-834.	1.7	17
36	Ab initio quantum chemical study of the formation, decomposition and isomerization of the formaldiminoxy radical (CH 2 NO): comparison of the Gaussian-2 and CASPT2 techniques in the calculation of potential energy surfaces. Theoretical Chemistry Accounts, 1998, 100, 212-221.	1.4	16

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37	Reactions of Phosphorus-Containing Species of Importance in the Catalytic Recombination of H + OH:Â Quantum Chemical and Kinetic Studiesâ€. Journal of Physical Chemistry A, 2002, 106, 10825-10830.	2.5	16
38	Covalent Bonding in the Hydrogen Molecule. Journal of Physical Chemistry A, 2017, 121, 9330-9345.	2.5	15
39	Hole localization and broken symmetry: A theoretical study of core electron ionization in the Li2 molecule. International Journal of Quantum Chemistry, 1987, 31, 471-487.	2.0	13
40	Quantum Chemical Determination of the Equilibrium Geometries and Harmonic Vibrational Frequencies of 1,1â€˜-, 1,2â€˜- and 2,2â€˜-Binaphthyl in Their Ground and Excited (1La) Electronic States. Journal of Physical Chemistry A, 2004, 108, 172-184.	2.5	13
41	Theoretical study of â€œprotonated pyruvateâ€• A methylhydroxycarbene-carbon dioxide complex-implications for the decarboxylation of pyruvic acid. Journal of Computational Chemistry, 1993, 14, 699-714.	3.3	12
42	Stereochemical and conformational consequences of the oxidation of 1,4-thiazane-3,5-dicarboxylates. Perkin Transactions II RSC, 2002, , 1066-1071.	1.1	9
43	The Mechanism of Covalent Bonding: Analysis within the HÃ¼ckel Model of Electronic Structure. Journal of Chemical Education, 2007, 84, 1201.	2.3	9
44	The absorbing boundary method for the calculation of quantum state decay rates. I. Numerical implementation and verification. Journal of Chemical Physics, 1979, 70, 2497-2510.	3.0	7
45	Quantum chemical characterization of the $${ilde{X}}(^{1} A_{1})$$ X ~ (1 A 1) , $${ilde{a}}(^{3}) Tj ETQq1 1 0.784314 rgBT /Over iodomethylidyne. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	7
46	Spectroscopy and heats of formation of CXI (X = Br, Cl, F) iodocarbenes: quantum chemical characterisation of the Xlf(¹ Aâ€²), Ã£(³ Aâ€³) and Ãf(¹ Aâ€³) states. Molecular Physics, 2015, 113, 1608-1617.	1.7	7
47	The Pyrolysis of 3â€Picoline: Ab Initio Quantum Chemical and Experimental (Shock Tube) Kinetic Studies. Israel Journal of Chemistry, 1996, 36, 239-248.	2.3	6
48	Orbital contraction and covalent bonding. Journal of Chemical Physics, 2022, 156, .	3.0	5
49	The absorbing boundary method. III. Tunneling decay and scattering resonances. Journal of Chemical Physics, 1980, 72, 2120-2130.	3.0	4
50	NMR resonance splitting of urea in stretched hydrogels: Proton exchange and 1 H/ 2 H isotopologues. Journal of Magnetic Resonance, 2014, 247, 72-80.	2.1	4
51	Protonation-Induced Paramagnetism. Structures and Stabilities of Six- and Seven-Coordinate Complexes of Os(II) in Singlet and Triplet States:Â A Density Functional Study. Journal of the American Chemical Society, 2001, 123, 5495-5506.	13.7	3
52	Structure and Bonding in Molecular Hydrogen Complexes of Osmium(II). Advances in Chemistry Series, 1997, , 21-38.	0.6	2
53	The Basics of Covalent Bonding. Journal of Chemical Education, 1997, 74, 1503.	2.3	1
54	The structure of N Î´-(N â€²-sulfodiaminophosphinyl)- l -ornithine and its binding to ornithine transcarbamoylase: A quantum chemical study. Molecular Simulation, 2002, 28, 773-790.	2.0	1