George C Shields

List of Publications by Year
in descending order

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105 papers	7,480 citations	87723 38 h-index	54797 84 g-index
108 all docs	108 docs citations	108 times ranked	5697 citing authors

#	Article	IF	Citations
1	Hydrogen-Bond Topology Is More Important Than Acid/Base Strength in Atmospheric Prenucleation Clusters. Journal of Physical Chemistry A, 2022, 126, 1718-1728.	1.1	19
2	Photochemistry and Photophysics of Charge-Transfer Excited States in Emissive d¹⁰/d⁰ Heterobimetallic Titanocene Tweezer Complexes. Inorganic Chemistry, 2022, 61, 10986-10998.	1.9	9
3	Insights into the charge-transfer character of electronic transitions in^RCp₂Ti(C₂Fc)₂complexes using solvatochromism, resonance Raman spectroscopy, and TDDFT. Dalton Transactions, 2021, 50, 2233-2242.	1.6	5
4	Calculating Reliable Gibbs Free Energies for Formation of Gas-Phase Clusters that Are Critical for Atmospheric Chemistry: (H2SO4)3. Journal of Physical Chemistry A, 2021, 125, 3169-3176.	1.1	22
5	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie, 2021, 133, 17031-17036.	1.6	0
6	The Role of Nonâ€Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. Angewandte Chemie - International Edition, 2021, 60, 16894-16899.	7.2	12
7	Monomers of Glycine and Serine Have a Limited Ability to Hydrate in the Atmosphere. Journal of Physical Chemistry A, 2021, 125, 8454-8467.	1.1	12
8	Ligand-to-Metal Charge-Transfer Photophysics and Photochemistry of Emissive d⁰ Titanocenes: A Spectroscopic and Computational Investigation. Inorganic Chemistry, 2021, 60, 14399-14409.	1.9	17
9	Particle formation and surface processes on atmospheric aerosols: A review of applied quantum chemical calculations. International Journal of Quantum Chemistry, 2020, 120, e26350.	1.0	30
10	Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances. International Journal of Quantum Chemistry, 2020, 120, e26370.	1.0	4
11	Catalytic activity of water molecules in gasâ€phase glycine dimerization. International Journal of Quantum Chemistry, 2020, 120, e26469.	1.0	11
12	Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational <scp>chemistry</scp> (<scp>MERCURY</scp>). International Journal of Quantum Chemistry, 2020, 120, e26274.	1.0	19
13	Water-Mediated Peptide Bond Formation in the Gas Phase: A Model Prebiotic Reaction. Journal of Physical Chemistry A, 2020, 124, 4150-4159.	1.1	16
14	The Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY): Twenty Years of Exceptional Success Supporting Undergraduate Research and Inclusive Excellence. Scholarship and Practice of Undergraduate Research, 2020, 3, 5-15.	0.2	10
15	Computation of Atmospheric Concentrations of Molecular Clusters from ab initio Thermochemistry. Journal of Visualized Experiments, 2020, , .	0.2	14
16	Water induces the same crown shapes as Li⁺ or Na⁺ in 15-crown-5 ether: a broadband rotational study. Physical Chemistry Chemical Physics, 2019, 21, 2875-2881.	1.3	20
17	Exploring the Rich Potential Energy Surface of (H₂O)₁₁ and Its Physical Implications. Journal of Chemical Theory and Computation, 2018, 14, 1141-1153.	2.3	20
18	Effect of Mixing Ammonia and Alkylamines on Sulfate Aerosol Formation. Journal of Physical Chemistry A, 2018, 122, 1612-1622.	1.1	54

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19	A Roadmap to Successful Collaborations between Primarily Undergraduate Institutions and Research Institutions. ACS Symposium Series, 2018, , 105-127.	0.5	6
20	ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhnâ€“Munkres Algorithm. Journal of Chemical Information and Modeling, 2017, 57, 1045-1054.	2.5	48
21	Corannulene and its complex with water: a tiny cup of water. Physical Chemistry Chemical Physics, 2017, 19, 14214-14223.	1.3	39
22	Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene. Journal of Physical Chemistry Letters, 2017, 8, 5744-5750.	2.1	48
23	Using Early Introduction to Research To Increase STEM Majors: A Tale of Two Colleges, One Small Highly Selective Private and One Non-Selective Regional Public. ACS Symposium Series, 2017, , 107-119.	0.5	2
24	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. Science, 2016, 351, 1310-1313.	6.0	256
25	Computational estimation of pK_a values. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2015, 5, 290-297.	6.2	85
26	Importance and Reliability of Small Basis Set CCSD(T) Corrections to MP2 Binding and Relative Energies of Water Clusters. Journal of Chemical Theory and Computation, 2015, 11, 1439-1448.	2.3	25
27	Formation of deprotonated 2-imidazoline-4(5)-one product ions in the collision-induced dissociation of some serine-containing dipeptides. International Journal of Mass Spectrometry, 2015, 381-382, 25-32.	0.7	1
28	Hydrogen Bond Cooperativity and the Threeâ€Đimensional Structures of Water Nonamers and Decamers. Angewandte Chemie - International Edition, 2014, 53, 14368-14372.	7.2	106
29	Structural Analysis of Î±-Fetoprotein (AFP)-like Peptides with Anti-Breast-Cancer Properties. Journal of Physical Chemistry B, 2014, 118, 4514-4526.	1.2	15
30	Hydration of the Sulfuric Acidâ€“Methylamine Complex and Implications for Aerosol Formation. Journal of Physical Chemistry A, 2014, 118, 7430-7441.	1.1	53
31	A Departmental Focus on High Impact Undergraduate Research Experiences. ACS Symposium Series, 2013, , 5-22.	0.5	8
32	Structure and thermodynamics of H3O+(H2O)8 clusters: A combined molecular dynamics and quantum mechanics approach. Computational and Theoretical Chemistry, 2013, 1021, 240-248.	1.1	13
33	Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. Chemical Physics Letters, 2013, 571, 1-15.	1.2	216
34	Quantum Mechanical Study of Sulfuric Acid Hydration: Atmospheric Implications. Journal of Physical Chemistry A, 2012, 116, 2209-2224.	1.1	111
35	Structures of Cage, Prism, and Book Isomers of Water Hexamer from Broadband Rotational Spectroscopy. Science, 2012, 336, 897-901.	6.0	377
36	Hydration of the Bisulfate Ion: Atmospheric Implications. Journal of Physical Chemistry A, 2012, 116, 5151-5163.	1.1	65

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37	Computational Study of the Hydration of Sulfuric Acid Dimers: Implications for Acid Dissociation and Aerosol Formation. Journal of Physical Chemistry A, 2012, 116, 9745-9758.	1.1	91
38	The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. Journal of Chemical Theory and Computation, 2011, 7, 2804-2817.	2.3	87
39	Benchmark Structures and Binding Energies of Small Water Clusters with Anharmonicity Corrections. Journal of Physical Chemistry A, 2011, 115, 12034-12046.	1.1	277
40	Atmospheric Implications for Formation of Clusters of Ammonium and 1â^'10 Water Molecules. Journal of Physical Chemistry A, 2010, 114, 4266-4271.	1.1	41
41	Accurate Predictions of Water Cluster Formation, (H₂O)_{n=2â^'10}. Journal of Physical Chemistry A, 2010, 114, 11725-11737.	1.1	213
42	Theoretical Calculations of Acid Dissociation Constants: A Review Article. Annual Reports in Computational Chemistry, 2010, , 113-138.	0.9	160
43	Ramachandranâ€type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. Journal of Computational Chemistry, 2009, 30, 910-921.	1.5	38
44	Antiestrogenic and anticancer activities of peptides derived from the active site of alphaâ€fetoprotein. Journal of Peptide Science, 2009, 15, 319-325.	0.8	14
45	Computational approaches for the design of peptides with anti-breast cancer properties. Future Medicinal Chemistry, 2009, 1, 201-212.	1.1	6
46	The Limitations of Certain Density Functionals in Modeling Neutral Water Clusters. Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry, 2008, 38, 32-39.	0.6	45
47	Thermodynamics of the Hydroxyl Radical Addition to Isoprene. Journal of Physical Chemistry A, 2008, 112, 7064-7071.	1.1	31
48	Hydration of OCS with One to Four Water Molecules in Atmospheric and Laboratory Conditions. Journal of Physical Chemistry A, 2008, 112, 4490-4495.	1.1	27
49	Experimental and Theoretical Study of the OH Vibrational Spectra and Overtone Chemistry of Gas-Phase Vinylacetic Acid. Journal of Physical Chemistry A, 2008, 112, 10226-10235.	1.1	24
50	Efficient and Accurate Characterization of the Bergman Cyclization for Several Enediynes Including an Expanded Substructure of Esperamicin A1. Journal of Physical Chemistry B, 2008, 112, 16917-16934.	1.2	18
51	In search of CS2(H2O)n=1â€“4 clusters. Journal of Chemical Physics, 2007, 126, 154320.	1.2	20
52	Computational Design and Experimental Discovery of an Antiestrogenic Peptide Derived from Î±-Fetoprotein. Journal of the American Chemical Society, 2007, 129, 6263-6268.	6.6	26
53	The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. International Journal of Quantum Chemistry, 2007, 107, 3001-3012.	1.0	12
54	Prediction of Accurate Anharmonic Experimental Vibrational Frequencies for Water Clusters, (H2O)n, n = 2â^'5. Journal of Physical Chemistry A, 2006, 110, 303-309.	1.1	99

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55	Exploration of the Potential Energy Surfaces, Prediction of Atmospheric Concentrations, and Prediction of Vibrational Spectra for the HO2Â·Â·Â·(H2O)n(n= 1â^'2) Hydrogen Bonded Complexes. Journal of Physical Chemistry A, 2006, 110, 3686-3691.	1.1	39
56	Ortho Effect in the Bergman Cyclization:â€‰ Electronic and Steric Effects in Hydrogen Abstraction by 1-Substituted Naphthalene 5,8-Diradicals. Journal of Physical Chemistry A, 2006, 110, 2517-2526.	1.1	48
57	Do Hydroxyl Radicalâ^'Water Clusters, OH(H2O)n,n= 1â^'5, Exist in the Atmosphere?. Journal of Physical Chemistry A, 2006, 110, 13283-13289.	1.1	93
58	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. International Journal of Quantum Chemistry, 2006, 106, 3122-3128.	1.0	29
59	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. Journal of Computational Chemistry, 2005, 26, 980-986.	1.5	50
60	Pople's Gaussian-3 model chemistry applied to an investigation of (H2O)8water clusters. International Journal of Quantum Chemistry, 2005, 102, 565-572.	1.0	38
61	Comparison of density functional theory predictions of gas-phase deprotonation data. International Journal of Quantum Chemistry, 2005, 105, 580-587.	1.0	43
62	Comparison of Model Chemistry and Density Functional Theory Thermochemical Predictions with Experiment for Formation of Ionic Clusters of the Ammonium Cation Complexed with Water and Ammonia; Atmospheric Implications. Journal of Physical Chemistry A, 2005, 109, 4905-4910.	1.1	54
63	Global Search for Minimum Energy (H2O)n Clusters, n = 3â^'5. Journal of Physical Chemistry A, 2005, 109, 6773-6778.	1.1	89
64	Comparison of CBS-QB3, CBS-APNO, G2, and G3 thermochemical predictions with experiment for formation of ionic clusters of hydronium and hydroxide ions complexed with water. Journal of Chemical Physics, 2005, 122, 024302.	1.2	57
65	The ability of the Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO model chemistries to model the geometries of small water clusters. International Journal of Quantum Chemistry, 2004, 100, 1065-1070.	1.0	33
66	Thermodynamics of Forming Water Clusters at Various Temperatures and Pressures by Gaussian-2, Gaussian-3, Complete Basis Set-QB3, and Complete Basis Set-APNO Model Chemistries; Implications for Atmospheric Chemistry. Journal of the American Chemical Society, 2004, 126, 2647-2653.	6.6	155
67	Accurate Experimental Values for the Free Energies of Hydration of H+, OH-, and H3O+. Journal of Physical Chemistry A, 2004, 108, 3692-3694.	1.1	135
68	Absolute pKa Determinations for Substituted Phenols. Journal of the American Chemical Society, 2002, 124, 6421-6427.	6.6	519
69	Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data. Journal of Physical Chemistry A, 2001, 105, 10483-10487.	1.1	131
70	Accurate relative pK[sub a] calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. Journal of Chemical Physics, 2001, 114, 4595.	1.2	145
71	Accurate pKaCalculations for Carboxylic Acids Using Complete Basis Set and Gaussian-n Models Combined with CPCM Continuum Solvation Methods. Journal of the American Chemical Society, 2001, 123, 7314-7319.	6.6	544
72	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. Journal of Physical Chemistry B, 2001, 105, 8445-8451.	1.2	15

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73	Experimentation with different thermodynamic cycles used for pKa calculations on carboxylic acids using complete basis set and Gaussian-n models combined with CPCM continuum solvation methods. International Journal of Quantum Chemistry, 2001, 85, 727-741.	1.0	176
74	An ONIOM study of the Bergman reaction: a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. Chemical Physics Letters, 2001, 347, 505-511.	1.2	10
75	Molecular Dynamics Simulation of a PNAÂ·DNAÂ·PNA Triple Helix in Aqueous Solution. Journal of the American Chemical Society, 1998, 120, 5895-5904.	6.6	99
76	Comparison of Experimental and Theoretical Structures of a Transition State Analogue Used for the Induction of Anti-Cocaine Catalytic Antibodies. Journal of Physical Chemistry A, 1997, 101, 8526-8529.	1.1	28
77	Molecular Dynamics Simulations of the d(TÂ·AÂ·T) Triple Helix. Journal of the American Chemical Society, 1997, 119, 7463-7469.	6.6	160
78	Use of the Supermolecule Approach To Model the Syn and Anti Conformations of Solvated Cyclic 3â€˜,5â€˜-Adenosine Monophosphate. The Journal of Physical Chemistry, 1996, 100, 3293-3298.	2.9	21
79	Quantum mechanical investigation of cyclic 3â€²,5â€²-adenosine monophosphate, the second hormonal messenger. Computational and Theoretical Chemistry, 1996, 362, 297-304.	1.5	9
80	A Semiempirical Transition State Structure for the First Step in the Alkaline Hydrolysis of Cocaine. Comparison between the Transition State Structure, the Phosphonate Monoester Transition State Analog, and a Newly Designed Thiophosphonate Transition State Analog. Journal of Molecular Modeling, 1996, 2, 62-69.	0.8	23
81	Semiempirical study of the bergman reaction: Towards a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. International Journal of Quantum Chemistry, 1995, 56, 51-59.	1.0	2
82	Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. International Journal of Quantum Chemistry, 1995, 56, 83-93.	1.0	17
83	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. International Journal of Quantum Chemistry, 1995, 56, 103-112.	1.0	14
84	Hydrogen bonding of nucleotide base pairs: Application of thePM3 method. International Journal of Quantum Chemistry, 1994, 52, 95-107.	1.0	23
85	Quantum-Mechanical investigation of large water clusters. International Journal of Quantum Chemistry, 1994, 52, 349-360.	1.0	29
86	Using the Franck-Hertz Experiment To Illustrate Quantization: Energy States of the Neon Atom by Electron Impact. Journal of Chemical Education, 1994, 71, 466.	1.1	3
87	The Physical Chemistry Sequence at Liberal Arts Colleges: The Lake Forest College Approach. Journal of Chemical Education, 1994, 71, 951.	1.1	7
88	Ability of the PM3 quantum-mechanical method to modelintermolecular hydrogen bonding between neutral molecules. Journal of Computational Chemistry, 1993, 14, 89-104.	1.5	158
89	Modeling of magic water clusters (H2O)20 and (H2O)21H+ with the PM3 quantum-mechanical method. Journal of Computational Chemistry, 1993, 14, 1326-1332.	1.5	35
90	Experiment in quantization: Atomic line spectra. Journal of Chemical Education, 1992, 69, 329.	1.1	6

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91	AM1 and PM3 calculations of the potential energy surfaces for hydroxymethyl radical reactions with nitric oxide and nitrogen dioxide. The Journal of Physical Chemistry, 1991, 95, 5085-5089.	2.9	12
92	Crystal structure of a CAP-DNA complex: the DNA is bent by 90 degrees. Science, 1991, 253, 1001-1007.	6.0	1,189
93	Crystallization of Escherichia coli catabolite gene activator protein with its DNA binding site. Journal of Molecular Biology, 1990, 213, 159-166.	2.0	44
94	Charge transfer reactions of organic ions containing oxygen: Correlation between reaction energetics and cross sections. Organic Mass Spectrometry, 1987, 22, 64-69.	1.3	21
95	Doubly charged ion mass spectra of alkyl-substituted furans and pyrroles. Organic Mass Spectrometry, 1987, 22, 389-399.	1.3	5
96	Competition between single and double electron transfer in collisions of doubly charged molecular pyrrole ions with neutral pyrrole molecules. International Journal of Mass Spectrometry and Ion Processes, 1987, 79, 127-140.	1.9	3
97	Evidence for long-lived excited states of [CnH2]2+ carbodications. Organic Mass Spectrometry, 1986, 21, 69-75.	1.3	11
98	Sensitivity of charge transfer reactions to hydrocarbon ion structures. Organic Mass Spectrometry, 1986, 21, 137-149.	1.3	14
99	Polarizabilites of organic ions. Organic Mass Spectrometry, 1986, 21, 449-450.	1.3	1
100	Doubly-charged ethane ions: Solution to the dilemma of stability predicted by theory and instability observed in experiment. Organic Mass Spectrometry, 1986, 21, 479-483.	1.3	10
101	Doubly-charged gas phase cations. Theoretica Chimica Acta, 1986, 69, 147-159.	0.9	22
102	Molecular charge-transfer cross sections and their correlation with reactant ion structures. The Journal of Physical Chemistry, 1985, 89, 4027-4031.	2.9	13
103	Structures, energetics and fragmentation pathways of CnH22+ carbodications. International Journal of Mass Spectrometry and Ion Processes, 1985, 64, 315-333.	1.9	15
104	Double electron transfer reactions of CO22+ ions. Chemical Physics Letters, 1983, 101, 287-290.	1.2	4
105	Single- and double-electron transfer reactions of ground and metastable state Ar2+ions. Journal of Physics B: Atomic and Molecular Physics, 1983, 16, 3591-3607.	1.6	14