George C Shields

List of Publications by Year in Descending Order

107 papers	6,423 citations	37 h-index	79 g-index
108 ext. papers	6,932 ext. citations	5 avg, IF	5.82 L-index

#	Paper	IF	Citations
107	Hydrogen-Bond Topology Is More Important Than Acid/Base Strength in Atmospheric Prenucleation Clusters.. *Journal of Physical Chemistry A*, **2022**,	2.8	4
106	Calculating Reliable Gibbs Free Energies for Formation of Gas-Phase Clusters that Are Critical for Atmospheric Chemistry: (HSO). *Journal of Physical Chemistry A*, **2021**, 125, 3169-3176	2.8	7
105	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. *Angewandte Chemie*, **2021**, 133, 17031-17036	3.6	
104	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. *Angewandte Chemie - International Edition*, **2021**, 60, 16894-16899	16.4	6
103	Insights into the charge-transfer character of electronic transitions in CpTi(CFc) complexes using solvatochromism, resonance Raman spectroscopy, and TDDFT. *Dalton Transactions*, **2021**, 50, 2233-2242	4.3	2
102	Monomers of Glycine and Serine Have a Limited Ability to Hydrate in the Atmosphere. *Journal of Physical Chemistry A*, **2021**, 125, 8454-8467	2.8	2
101	Ligand-to-Metal Charge-Transfer Photophysics and Photochemistry of Emissive d Titanocenes: A Spectroscopic and Computational Investigation. *Inorganic Chemistry*, **2021**, 60, 14399-14409	5.1	2
100	Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY). *International Journal of Quantum Chemistry*, **2020**, 120, e26274	2.1	5
99	Water-Mediated Peptide Bond Formation in the Gas Phase: A Model Prebiotic Reaction. *Journal of Physical Chemistry A*, **2020**, 124, 4150-4159	2.8	6
98	The Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY): Twenty Years of Exceptional Success Supporting Undergraduate Research and Inclusive Excellence **2020**, 3, 5-15		5
97	Computation of Atmospheric Concentrations of Molecular Clusters from ab initio Thermochemistry. *Journal of Visualized Experiments*, **2020**,	1.6	10
96	Particle formation and surface processes on atmospheric aerosols: A review of applied quantum chemical calculations. *International Journal of Quantum Chemistry*, **2020**, 120, e26350	2.1	10
95	Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances. *International Journal of Quantum Chemistry*, **2020**, 120, e26370	2.1	1
94	Catalytic activity of water molecules in gas-phase glycine dimerization. *International Journal of Quantum Chemistry*, **2020**, 120, e26469	2.1	2
93	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	3.6	13
92	Exploring the Rich Potential Energy Surface of (HO) and Its Physical Implications. *Journal of Chemical Theory and Computation*, **2018**, 14, 1141-1153	6.4	15
91	Effect of Mixing Ammonia and Alkylamines on Sulfate Aerosol Formation. *Journal of Physical Chemistry A*, **2018**, 122, 1612-1622	2.8	40

90	A Roadmap to Successful Collaborations between Primarily Undergraduate Institutions and Research Institutions. *ACS Symposium Series*, **2018**, 105-127	0.4	3
89	ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhn-Munkres Algorithm. *Journal of Chemical Information and Modeling*, **2017**, 57, 1045-1054	6.1	32
88	Corannulene and its complex with water: a tiny cup of water. *Physical Chemistry Chemical Physics*, **2017**, 19, 14214-14223	3.6	30
87	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	6.4	30
86	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	0.4	2
85	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. *Science*, **2016**, 351, 1310-3	33.3	182
84	Guest Foreword. *ACS Symposium Series*, **2016**, xiii-xv	0.4	1
83	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, 1439-48	6.4	20
82	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	1.9	1
81	Computational estimation of pKa values. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2015**, 5, 290-297	7.9	58
80	Hydrogen bond cooperativity and the three-dimensional structures of water nonamers and decamers. *Angewandte Chemie - International Edition*, **2014**, 53, 14368-72	16.4	82
79	Structural analysis of Ffetoprotein (AFP)-like peptides with anti-breast-cancer properties. *Journal of Physical Chemistry B*, **2014**, 118, 4514-26	3.4	13
78	Hydration of the sulfuric acid-methylamine complex and implications for aerosol formation. *Journal of Physical Chemistry A*, **2014**, 118, 7430-41	2.8	43
77	Hydrogen Bond Cooperativity and the Three-Dimensional Structures of Water Nonamers and Decamers. *Angewandte Chemie*, **2014**, 126, 14596-14600	3.6	7
76	A Departmental Focus on High Impact Undergraduate Research Experiences. *ACS Symposium Series*, **2013**, 5-22	0.4	6
75	Structure and thermodynamics of H3O+(H2O)8 clusters: A combined molecular dynamics and quantum mechanics approach. *Computational and Theoretical Chemistry*, **2013**, 1021, 240-248	2	12
74	Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. *Chemical Physics Letters*, **2013**, 571, 1-15	2.5	166
73	Quantum mechanical study of sulfuric acid hydration: atmospheric implications. *Journal of Physical Chemistry A*, **2012**, 116, 2209-24	2.8	95

72	Structures of cage, prism, and book isomers of water hexamer from broadband rotational spectroscopy. *Science*, **2012**, 336, 897-901	33.3	318
71	Hydration of the bisulfate ion: atmospheric implications. *Journal of Physical Chemistry A*, **2012**, 116, 5151-63	2.8	55
70	Computational study of the hydration of sulfuric acid dimers: implications for acid dissociation and aerosol formation. *Journal of Physical Chemistry A*, **2012**, 116, 9745-58	2.8	74
69	The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. *Journal of Chemical Theory and Computation*, **2011**, 7, 2804-17	6.4	72
68	Benchmark structures and binding energies of small water clusters with anharmonicity corrections. *Journal of Physical Chemistry A*, **2011**, 115, 12034-46	2.8	234
67	Atmospheric implications for formation of clusters of ammonium and 1-10 water molecules. *Journal of Physical Chemistry A*, **2010**, 114, 4266-71	2.8	33
66	Accurate predictions of water cluster formation, (H□O)(n=2-10). *Journal of Physical Chemistry A*, **2010**, 114, 11725-37	2.8	183
65	Theoretical Calculations of Acid Dissociation Constants: A Review Article. *Annual Reports in Computational Chemistry*, **2010**, 113-138	1.8	125
64	Ramachandran-type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. *Journal of Computational Chemistry*, **2009**, 30, 910-21	3.5	31
63	Antiestrogenic and anticancer activities of peptides derived from the active site of alpha-fetoprotein. *Journal of Peptide Science*, **2009**, 15, 319-25	2.1	12
62	Computational approaches for the design of peptides with anti-breast cancer properties. *Future Medicinal Chemistry*, **2009**, 1, 201-12	4.1	6
61	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		41
60	Thermodynamics of the hydroxyl radical addition to isoprene. *Journal of Physical Chemistry A*, **2008**, 112, 7064-71	2.8	30
59	Hydration of OCS with one to four water molecules in atmospheric and laboratory conditions. *Journal of Physical Chemistry A*, **2008**, 112, 4490-5	2.8	26
58	Experimental and theoretical study of the OH vibrational spectra and overtone chemistry of gas-phase vinylacetic acid. *Journal of Physical Chemistry A*, **2008**, 112, 10226-35	2.8	23
57	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, 16917-34	3.4	14
56	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	2.1	11
55	In search of CS2(H2O)(n=1-4) clusters. *Journal of Chemical Physics*, **2007**, 126, 154320	3.9	20

54	Computational design and experimental discovery of an antiestrogenic peptide derived from alpha-fetoprotein. *Journal of the American Chemical Society*, **2007**, 129, 6263-8	16.4	23
53	Prediction of accurate anharmonic experimental vibrational frequencies for water clusters, (H2O)n, n=2-5. *Journal of Physical Chemistry A*, **2006**, 110, 303-9	2.8	89
52	Exploration of the potential energy surfaces, prediction of atmospheric concentrations, and prediction of vibrational spectra for the HO2...(H2O)n (n = 1-2) hydrogen bonded complexes. *Journal of Physical Chemistry A*, **2006**, 110, 3686-91	2.8	36
51	Ortho effect in the Bergman cyclization: electronic and steric effects in hydrogen abstraction by 1-substituted naphthalene 5,8-diradicals. *Journal of Physical Chemistry A*, **2006**, 110, 2517-26	2.8	43
50	Do hydroxyl radical-water clusters, OH(H2O)n, n = 1-5, exist in the atmosphere?. *Journal of Physical Chemistry A*, **2006**, 110, 13283-9	2.8	89
49	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. *International Journal of Quantum Chemistry*, **2006**, 106, 3122-3128	2.1	26
48	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, 4905-10	2.8	46
47	Global search for minimum energy (H2O)n clusters, n = 3-5. *Journal of Physical Chemistry A*, **2005**, 109, 6773-8	2.8	83
46	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	3.9	50
45	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. *Journal of Computational Chemistry*, **2005**, 26, 980-6	3.5	47
44	Pople Gaussian-3 model chemistry applied to an investigation of (H2O)8 water clusters. *International Journal of Quantum Chemistry*, **2005**, 102, 565-572	2.1	37
43	Comparison of density functional theory predictions of gas-phase deprotonation data. *International Journal of Quantum Chemistry*, **2005**, 105, 580-587	2.1	38
42	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	2.1	31
41	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, 2647-53	16.4	134
40	Accurate Experimental Values for the Free Energies of Hydration of H+, OH-, and H3O+. *Journal of Physical Chemistry A*, **2004**, 108, 3692-3694	2.8	124
39	Absolute pK(a) determinations for substituted phenols. *Journal of the American Chemical Society*, **2002**, 124, 6421-7	16.4	468
38	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	2.1	163
37	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	2.5	8

36	Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data. *Journal of Physical Chemistry A*, **2001**, 105, 10483-10487	2.8	120
35	Accurate relative pKa calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. *Journal of Chemical Physics*, **2001**, 114, 4595	3.9	133
34	Accurate pK(a) calculations 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, 7314-9	16.4	494
33	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. *Journal of Physical Chemistry B*, **2001**, 105, 8445-8451	3.4	15
32	Molecular Dynamics Simulation of a PNA·DNA·PNA Triple Helix in Aqueous Solution. *Journal of the American Chemical Society*, **1998**, 120, 5895-5904	16.4	94
31	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	2.8	24
30	Molecular Dynamics Simulations of the d(T·A·T) Triple Helix. *Journal of the American Chemical Society*, **1997**, 119, 7463-7469	16.4	156
29	Use of the Supermolecule Approach To Model the Syn and Anti Conformations of Solvated Cyclic 3′,5′-Adenosine Monophosphate. *The Journal of Physical Chemistry*, **1996**, 100, 3293-3298		17
28	Quantum mechanical investigation of cyclic 3?,5?-adenosine monophosphate, the second hormonal messenger. *Computational and Theoretical Chemistry*, **1996**, 362, 297-304		8
27	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	2	20
26	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	2.1	2
25	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	2.1	14
24	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. *International Journal of Quantum Chemistry*, **1995**, 56, 103-112	2.1	12
23	Hydrogen bonding of nucleotide base pairs: Application of the PM3 method. *International Journal of Quantum Chemistry*, **1994**, 52, 95-107	2.1	23
22	Quantum-Mechanical investigation of large water clusters. *International Journal of Quantum Chemistry*, **1994**, 52, 349-360	2.1	27
21	Using the Franck-Hertz Experiment To Illustrate Quantization: Energy States of the Neon Atom by Electron Impact. *Journal of Chemical Education*, **1994**, 71, 466	2.4	2
20	The Physical Chemistry Sequence at Liberal Arts Colleges: The Lake Forest College Approach. *Journal of Chemical Education*, **1994**, 71, 951	2.4	7
19	Ability of the PM3 quantum-mechanical method to model intermolecular hydrogen bonding between neutral molecules. *Journal of Computational Chemistry*, **1993**, 14, 89-104	3.5	145

18	Modeling of magic water clusters (H2O)20 and (H2O)21H+ with the PM3 quantum-mechanical method. *Journal of Computational Chemistry*, **1993**, 14, 1326-1332	3.5	33
17	Experiment in quantization: Atomic line spectra. *Journal of Chemical Education*, **1992**, 69, 329	2.4	5
16	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		9
15	Crystal structure of a CAP-DNA complex: the DNA is bent by 90 degrees. *Science*, **1991**, 253, 1001-7	33.3	1092
14	Crystallization of Escherichia coli catabolite gene activator protein with its DNA binding site. The use of modular DNA. *Journal of Molecular Biology*, **1990**, 213, 159-66	6.5	41
13	Charge transfer reactions of organic ions containing oxygen: Correlation between reaction energetics and cross sections. *Organic Mass Spectrometry*, **1987**, 22, 64-69		21
12	Doubly charged ion mass spectra of alkyl-substituted furans and pyrroles. *Organic Mass Spectrometry*, **1987**, 22, 389-399		5
11	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		3
10	Evidence for long-lived excited states of [CnH2]2+ carbodications. *Organic Mass Spectrometry*, **1986**, 21, 69-75		11
9	Sensitivity of charge transfer reactions to hydrocarbon ion structures. *Organic Mass Spectrometry*, **1986**, 21, 137-149		14
8	Polarizabilites of organic ions. *Organic Mass Spectrometry*, **1986**, 21, 449-450		1
7	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		10
6	Doubly-charged gas phase cations. *Theoretica Chimica Acta*, **1986**, 69, 147-159		21
5	Molecular charge-transfer cross sections and their correlation with reactant ion structures. *The Journal of Physical Chemistry*, **1985**, 89, 4027-4031		12
4	Structures, energetics and fragmentation pathways of CnH22+ carbodications. *International Journal of Mass Spectrometry and Ion Processes*, **1985**, 64, 315-333		15
3	Double electron transfer reactions of CO22+ ions. *Chemical Physics Letters*, **1983**, 101, 287-290	2.5	4
2	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		12
1	Computational Approaches for the Prediction of pKa Values		44