

# George C Shields

## List of Publications by Citations

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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	Crystal structure of a CAP-DNA complex: the DNA is bent by 90 degrees. <i>Science</i> , <b>1991</b> , 253, 1001-7	33.3	1092
106	Accurate pK(a) calculations for carboxylic acids using complete basis set and Gaussian-n models combined with CPCM continuum solvation methods. <i>Journal of the American Chemical Society</i> , <b>2001</b> , 123, 7314-9	16.4	494
105	Absolute pK(a) determinations for substituted phenols. <i>Journal of the American Chemical Society</i> , <b>2002</b> , 124, 6421-7	16.4	468
104	Structures of cage, prism, and book isomers of water hexamer from broadband rotational spectroscopy. <i>Science</i> , <b>2012</b> , 336, 897-901	33.3	318
103	Benchmark structures and binding energies of small water clusters with anharmonicity corrections. <i>Journal of Physical Chemistry A</i> , <b>2011</b> , 115, 12034-46	2.8	234
102	Accurate predictions of water cluster formation, (H <sub>2</sub> O) <sub>n</sub> (n=2-10). <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 11725-37	2.8	183
101	Concerted hydrogen-bond breaking by quantum tunneling in the water hexamer prism. <i>Science</i> , <b>2016</b> , 351, 1310-3	33.3	182
100	Broadband Fourier transform rotational spectroscopy for structure determination: The water heptamer. <i>Chemical Physics Letters</i> , <b>2013</b> , 571, 1-15	2.5	166
99	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. <i>International Journal of Quantum Chemistry</i> , <b>2001</b> , 85, 727-741	2.1	163
98	Molecular Dynamics Simulations of the d(TAAT) Triple Helix. <i>Journal of the American Chemical Society</i> , <b>1997</b> , 119, 7463-7469	16.4	156
97	Ability of the PM3 quantum-mechanical method to model intermolecular hydrogen bonding between neutral molecules. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 89-104	3.5	145
96	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. <i>Journal of the American Chemical Society</i> , <b>2004</b> , 126, 2647-53	16.4	134
95	Accurate relative pKa calculations for carboxylic acids using complete basis set and Gaussian-n models combined with continuum solvation methods. <i>Journal of Chemical Physics</i> , <b>2001</b> , 114, 4595	3.9	133
94	Theoretical Calculations of Acid Dissociation Constants: A Review Article. <i>Annual Reports in Computational Chemistry</i> , <b>2010</b> , 113-138	1.8	125
93	Accurate Experimental Values for the Free Energies of Hydration of H <sup>+</sup> , OH <sup>-</sup> , and H <sub>3</sub> O <sup>+</sup> . <i>Journal of Physical Chemistry A</i> , <b>2004</b> , 108, 3692-3694	2.8	124
92	Comparison of CBS-QB3, CBS-APNO, and G3 Predictions of Gas Phase Deprotonation Data. <i>Journal of Physical Chemistry A</i> , <b>2001</b> , 105, 10483-10487	2.8	120
91	Quantum mechanical study of sulfuric acid hydration: atmospheric implications. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 2209-24	2.8	95

90	Molecular Dynamics Simulation of a PNA-DNA-PNA Triple Helix in Aqueous Solution. <i>Journal of the American Chemical Society</i> , <b>1998</b> , 120, 5895-5904	16.4	94
89	Prediction of accurate anharmonic experimental vibrational frequencies for water clusters, (H <sub>2</sub> O) <sub>n</sub> , n=2-5. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 303-9	2.8	89
88	Do hydroxyl radical-water clusters, OH(H <sub>2</sub> O) <sub>n</sub> , n = 1-5, exist in the atmosphere?. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 13283-9	2.8	89
87	Global search for minimum energy (H <sub>2</sub> O) <sub>n</sub> clusters, n = 3-5. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 6773-8	2.8	83
86	Hydrogen bond cooperativity and the three-dimensional structures of water nonamers and decamers. <i>Angewandte Chemie - International Edition</i> , <b>2014</b> , 53, 14368-72	16.4	82
85	Computational study of the hydration of sulfuric acid dimers: implications for acid dissociation and aerosol formation. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 9745-58	2.8	74
84	The Role of Anharmonicity in Hydrogen-Bonded Systems: The Case of Water Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2011</b> , 7, 2804-17	6.4	72
83	Computational estimation of pKa values. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , <b>2015</b> , 5, 290-297	7.9	58
82	Hydration of the bisulfate ion: atmospheric implications. <i>Journal of Physical Chemistry A</i> , <b>2012</b> , 116, 5151-55	12.63	55
81	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. <i>Journal of Chemical Physics</i> , <b>2005</b> , 122, 024302	3.9	50
80	First-principle studies of intermolecular and intramolecular catalysis of protonated cocaine. <i>Journal of Computational Chemistry</i> , <b>2005</b> , 26, 980-6	3.5	47
79	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. <i>Journal of Physical Chemistry A</i> , <b>2005</b> , 109, 4905-10	2.8	46
78	Computational Approaches for the Prediction of pKa Values		44
77	Hydration of the sulfuric acid-methylamine complex and implications for aerosol formation. <i>Journal of Physical Chemistry A</i> , <b>2014</b> , 118, 7430-41	2.8	43
76	Ortho effect in the Bergman cyclization: electronic and steric effects in hydrogen abstraction by 1-substituted naphthalene 5,8-diradicals. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 2517-26	2.8	43
75	The Limitations of Certain Density Functionals in Modeling Neutral Water Clusters. <i>Synthesis and Reactivity in Inorganic, Metal Organic, and Nano Metal Chemistry</i> , <b>2008</b> , 38, 32-39		41
74	Crystallization of Escherichia coli catabolite gene activator protein with its DNA binding site. The use of modular DNA. <i>Journal of Molecular Biology</i> , <b>1990</b> , 213, 159-66	6.5	41
73	Effect of Mixing Ammonia and Alkylamines on Sulfate Aerosol Formation. <i>Journal of Physical Chemistry A</i> , <b>2018</b> , 122, 1612-1622	2.8	40

72	Comparison of density functional theory predictions of gas-phase deprotonation data. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 105, 580-587	2.1	38
71	PopleQ Gaussian-3 model chemistry applied to an investigation of (H <sub>2</sub> O) <sub>8</sub> water clusters. <i>International Journal of Quantum Chemistry</i> , <b>2005</b> , 102, 565-572	2.1	37
70	Exploration of the potential energy surfaces, prediction of atmospheric concentrations, and prediction of vibrational spectra for the HO <sub>2</sub> ...(H <sub>2</sub> O) <sub>n</sub> (n = 1-2) hydrogen bonded complexes. <i>Journal of Physical Chemistry A</i> , <b>2006</b> , 110, 3686-91	2.8	36
69	Atmospheric implications for formation of clusters of ammonium and 1-10 water molecules. <i>Journal of Physical Chemistry A</i> , <b>2010</b> , 114, 4266-71	2.8	33
68	Modeling of magic water clusters (H <sub>2</sub> O) <sub>20</sub> and (H <sub>2</sub> O) <sub>21</sub> H <sup>+</sup> with the PM3 quantum-mechanical method. <i>Journal of Computational Chemistry</i> , <b>1993</b> , 14, 1326-1332	3.5	33
67	ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhn-Munkres Algorithm. <i>Journal of Chemical Information and Modeling</i> , <b>2017</b> , 57, 1045-1054	6.1	32
66	Ramachandran-type plots for glycosidic linkages: Examples from molecular dynamic simulations using the Glycam06 force field. <i>Journal of Computational Chemistry</i> , <b>2009</b> , 30, 910-21	3.5	31
65	The ability of the Gaussian-2, Gaussian-3, Complete Basis SetQ3, and Complete Basis SetAPNO model chemistries to model the geometries of small water clusters. <i>International Journal of Quantum Chemistry</i> , <b>2004</b> , 100, 1065-1070	2.1	31
64	Corannulene and its complex with water: a tiny cup of water. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 14214-14223	3.6	30
63	Capturing the Elusive Water Trimer from the Stepwise Growth of Water on the Surface of the Polycyclic Aromatic Hydrocarbon Acenaphthene. <i>Journal of Physical Chemistry Letters</i> , <b>2017</b> , 8, 5744-5750	6.4	30
62	Thermodynamics of the hydroxyl radical addition to isoprene. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 7064-71	2.8	30
61	Quantum-Mechanical investigation of large water clusters. <i>International Journal of Quantum Chemistry</i> , <b>1994</b> , 52, 349-360	2.1	27
60	Hydration of OCS with one to four water molecules in atmospheric and laboratory conditions. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 4490-5	2.8	26
59	CCSD(T), W1, and other model chemistry predictions for gas-phase deprotonation reactions. <i>International Journal of Quantum Chemistry</i> , <b>2006</b> , 106, 3122-3128	2.1	26
58	Comparison of Experimental and Theoretical Structures of a Transition State Analogue Used for the Induction of Anti-Cocaine Catalytic Antibodies. <i>Journal of Physical Chemistry A</i> , <b>1997</b> , 101, 8526-8529	2.8	24
57	Experimental and theoretical study of the OH vibrational spectra and overtone chemistry of gas-phase vinylacetic acid. <i>Journal of Physical Chemistry A</i> , <b>2008</b> , 112, 10226-35	2.8	23
56	Computational design and experimental discovery of an antiestrogenic peptide derived from alpha-fetoprotein. <i>Journal of the American Chemical Society</i> , <b>2007</b> , 129, 6263-8	16.4	23
55	Hydrogen bonding of nucleotide base pairs: Application of the PM3 method. <i>International Journal of Quantum Chemistry</i> , <b>1994</b> , 52, 95-107	2.1	23

54	Doubly-charged gas phase cations. <i>Theoretica Chimica Acta</i> , <b>1986</b> , 69, 147-159		21
53	Charge transfer reactions of organic ions containing oxygen: Correlation between reaction energetics and cross sections. <i>Organic Mass Spectrometry</i> , <b>1987</b> , 22, 64-69		21
52	Importance and Reliability of Small Basis Set CCSD(T) Corrections to MP2 Binding and Relative Energies of Water Clusters. <i>Journal of Chemical Theory and Computation</i> , <b>2015</b> , 11, 1439-48	6.4	20
51	In search of CS <sub>2</sub> (H <sub>2</sub> O)(n=1-4) clusters. <i>Journal of Chemical Physics</i> , <b>2007</b> , 126, 154320	3.9	20
50	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. <i>Journal of Molecular Modeling</i> , <b>1996</b> , 2, 62-69	2	20
49	Use of the Supermolecule Approach To Model the Syn and Anti Conformations of Solvated Cyclic 3'-[5'-Adenosine Monophosphate. <i>The Journal of Physical Chemistry</i> , <b>1996</b> , 100, 3293-3298		17
48	Exploring the Rich Potential Energy Surface of (HO) and Its Physical Implications. <i>Journal of Chemical Theory and Computation</i> , <b>2018</b> , 14, 1141-1153	6.4	15
47	Further Quantum Mechanical Evidence that Difluorotoluene Does Not Hydrogen Bond. <i>Journal of Physical Chemistry B</i> , <b>2001</b> , 105, 8445-8451	3.4	15
46	Structures, energetics and fragmentation pathways of C <sub>n</sub> H <sub>22</sub> <sup>+</sup> carbocations. <i>International Journal of Mass Spectrometry and Ion Processes</i> , <b>1985</b> , 64, 315-333		15
45	Efficient and accurate characterization of the Bergman cyclization for several enediynes including an expanded substructure of esperamicin A1. <i>Journal of Physical Chemistry B</i> , <b>2008</b> , 112, 16917-34	3.4	14
44	Investigation of the potential energy surface for the first step in the alkaline hydrolysis of methyl acetate. <i>International Journal of Quantum Chemistry</i> , <b>1995</b> , 56, 83-93	2.1	14
43	Sensitivity of charge transfer reactions to hydrocarbon ion structures. <i>Organic Mass Spectrometry</i> , <b>1986</b> , 21, 137-149		14
42	Water induces the same crown shapes as Li or Na in 15-crown-5 ether: a broadband rotational study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 2875-2881	3.6	13
41	Structural analysis of α-fetoprotein (AFP)-like peptides with anti-breast-cancer properties. <i>Journal of Physical Chemistry B</i> , <b>2014</b> , 118, 4514-26	3.4	13
40	Structure and thermodynamics of H <sub>3</sub> O <sup>+</sup> (H <sub>2</sub> O) <sub>8</sub> clusters: A combined molecular dynamics and quantum mechanics approach. <i>Computational and Theoretical Chemistry</i> , <b>2013</b> , 1021, 240-248	2	12
39	Antiestrogenic and anticancer activities of peptides derived from the active site of alpha-fetoprotein. <i>Journal of Peptide Science</i> , <b>2009</b> , 15, 319-25	2.1	12
38	A computationally efficient procedure for modeling the first step in the alkaline hydrolysis of esters. <i>International Journal of Quantum Chemistry</i> , <b>1995</b> , 56, 103-112	2.1	12
37	Single- and double-electron transfer reactions of ground and metastable state Ar <sub>2</sub> <sup>+</sup> ions. <i>Journal of Physics B: Atomic and Molecular Physics</i> , <b>1983</b> , 16, 3591-3607		12

36	Molecular charge-transfer cross sections and their correlation with reactant ion structures. <i>The Journal of Physical Chemistry</i> , <b>1985</b> , 89, 4027-4031		12
35	The search for low energy conformational families of small peptides: Searching for active conformations of small peptides in the absence of a known receptor. <i>International Journal of Quantum Chemistry</i> , <b>2007</b> , 107, 3001-3012	2.1	11
34	Evidence for long-lived excited states of $[C_nH_2]^{2+}$ carbocations. <i>Organic Mass Spectrometry</i> , <b>1986</b> , 21, 69-75		11
33	Doubly-charged ethane ions: Solution to the dilemma of stability predicted by theory and instability observed in experiment. <i>Organic Mass Spectrometry</i> , <b>1986</b> , 21, 479-483		10
32	Computation of Atmospheric Concentrations of Molecular Clusters from ab initio Thermochemistry. <i>Journal of Visualized Experiments</i> , <b>2020</b> ,	1.6	10
31	Particle formation and surface processes on atmospheric aerosols: A review of applied quantum chemical calculations. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26350	2.1	10
30	AM1 and PM3 calculations of the potential energy surfaces for hydroxymethyl radical reactions with nitric oxide and nitrogen dioxide. <i>The Journal of Physical Chemistry</i> , <b>1991</b> , 95, 5085-5089		9
29	An ONIOM study of the Bergman reaction: a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. <i>Chemical Physics Letters</i> , <b>2001</b> , 347, 505-511	2.5	8
28	Quantum mechanical investigation of cyclic 3',5'-adenosine monophosphate, the second hormonal messenger. <i>Computational and Theoretical Chemistry</i> , <b>1996</b> , 362, 297-304		8
27	Hydrogen Bond Cooperativity and the Three-Dimensional Structures of Water Nonamers and Decamers. <i>Angewandte Chemie</i> , <b>2014</b> , 126, 14596-14600	3.6	7
26	The Physical Chemistry Sequence at Liberal Arts Colleges: The Lake Forest College Approach. <i>Journal of Chemical Education</i> , <b>1994</b> , 71, 951	2.4	7
25	Calculating Reliable Gibbs Free Energies for Formation of Gas-Phase Clusters that Are Critical for Atmospheric Chemistry: (HSO). <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 3169-3176	2.8	7
24	Water-Mediated Peptide Bond Formation in the Gas Phase: A Model Prebiotic Reaction. <i>Journal of Physical Chemistry A</i> , <b>2020</b> , 124, 4150-4159	2.8	6
23	A Departmental Focus on High Impact Undergraduate Research Experiences. <i>ACS Symposium Series</i> , <b>2013</b> , 5-22	0.4	6
22	Computational approaches for the design of peptides with anti-breast cancer properties. <i>Future Medicinal Chemistry</i> , <b>2009</b> , 1, 201-12	4.1	6
21	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie - International Edition</i> , <b>2021</b> , 60, 16894-16899	16.4	6
20	Twenty years of exceptional success: The molecular education and research consortium in undergraduate computational chemistry (MERCURY). <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26274	2.1	5
19	Experiment in quantization: Atomic line spectra. <i>Journal of Chemical Education</i> , <b>1992</b> , 69, 329	2.4	5

18	Doubly charged ion mass spectra of alkyl-substituted furans and pyrroles. <i>Organic Mass Spectrometry</i> , <b>1987</b> , 22, 389-399		5
17	The Molecular Education and Research Consortium in Undergraduate Computational Chemistry (MERCURY): Twenty Years of Exceptional Success Supporting Undergraduate Research and Inclusive Excellence <b>2020</b> , 3, 5-15		5
16	Double electron transfer reactions of CO <sub>2</sub> <sup>+</sup> ions. <i>Chemical Physics Letters</i> , <b>1983</b> , 101, 287-290	2.5	4
15	Hydrogen-Bond Topology Is More Important Than Acid/Base Strength in Atmospheric Prenucleation Clusters.. <i>Journal of Physical Chemistry A</i> , <b>2022</b> ,	2.8	4
14	Competition between single and double electron transfer in collisions of doubly charged molecular pyrrole ions with neutral pyrrole molecules. <i>International Journal of Mass Spectrometry and Ion Processes</i> , <b>1987</b> , 79, 127-140		3
13	A Roadmap to Successful Collaborations between Primarily Undergraduate Institutions and Research Institutions. <i>ACS Symposium Series</i> , <b>2018</b> , 105-127	0.4	3
12	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. <i>ACS Symposium Series</i> , <b>2017</b> , 107-119	0.4	2
11	Semiempirical study of the bergman reaction: Towards a computationally efficient and accurate method for modeling the enediyne anticancer antibiotics. <i>International Journal of Quantum Chemistry</i> , <b>1995</b> , 56, 51-59	2.1	2
10	Using the Franck-Hertz Experiment To Illustrate Quantization: Energy States of the Neon Atom by Electron Impact. <i>Journal of Chemical Education</i> , <b>1994</b> , 71, 466	2.4	2
9	Catalytic activity of water molecules in gas-phase glycine dimerization. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26469	2.1	2
8	Insights into the charge-transfer character of electronic transitions in CpTi(CFc) complexes using solvatochromism, resonance Raman spectroscopy, and TDDFT. <i>Dalton Transactions</i> , <b>2021</b> , 50, 2233-2242 <sup>4,3</sup>		2
7	Monomers of Glycine and Serine Have a Limited Ability to Hydrate in the Atmosphere. <i>Journal of Physical Chemistry A</i> , <b>2021</b> , 125, 8454-8467	2.8	2
6	Ligand-to-Metal Charge-Transfer Photophysics and Photochemistry of Emissive d Titanocenes: A Spectroscopic and Computational Investigation. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 14399-14409	5.1	2
5	Formation of deprotonated 2-imidazoline-4(5)-one product ions in the collision-induced dissociation of some serine-containing dipeptides. <i>International Journal of Mass Spectrometry</i> , <b>2015</b> , 381-382, 25-32	1.9	1
4	Polarizabilities of organic ions. <i>Organic Mass Spectrometry</i> , <b>1986</b> , 21, 449-450		1
3	Maintaining a high degree of research productivity at a predominately undergraduate institution as your career advances. <i>International Journal of Quantum Chemistry</i> , <b>2020</b> , 120, e26370	2.1	1
2	Guest Foreword. <i>ACS Symposium Series</i> , <b>2016</b> , xiii-xv	0.4	1
1	The Role of Non-Covalent Interactions on Cluster Formation: Pentamer, Hexamers and Heptamer of Difluoromethane. <i>Angewandte Chemie</i> , <b>2021</b> , 133, 17031-17036	3.6	

